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Public reporting burden for this collection of information is estimated to average 1 hour per response, incligathering and maintaining the data needed, and completing and reviewing the collection of information. So of this ferson collection of information, including suggestions for reducing this burden, to Washington Headquarters Ser Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Pa				
1. AGENCY USE ONLY (Leave blan	2. REPORT DATE 13 Feb 02	3. REPOIL LIFE AND Final Repo		
4. TITLE AND SUBTITLE THE 2001 GORDON RESEARC TRANSFER			5. FUNDING NUMBERS F49620-00-1-0340 2303/EX	
6. AUTHOR(S) Mr Carlyle B. Storm			61102F	:
7. PERFORMING ORGANIZATION I Gordon Research Conferences In P.O. Box 984 West Kingston, RI 02892-0984			8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AG AFOSR/NL 801 N Randolph Street, Suite 732 Arlington VA 22203-1977		;)	10. SPONSORING/MONITORING AGENCY REPORT NUMBER	
11. SUPPLEMENTARY NOTES				
12a. DISTRIBUTION AVAILABILITY			12b. DISTRIBUTION CODE	
Approve for Public	c Release: Distribution	n Unlimited		
13. ABSTRACT (Maximum 200 words) The Gordon Research Conference (GRC) on Molecular Energy Transfer was held at Harbortown Resort, Ventura, California January 14-19, 2001. The conference was well attended with 89 participants (list enclosed). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both US and foreign scientists, senior researchers, young investigators, and students. In designing the formal speakers program, emphasis was placed on current unpublished research and discussion of the future target areas in this field. There was a conscious effort to stimulate lively discussion about the key issues in the field today. Time for formal presentations was limited in the interest of group discussions. In order that more scientists could communicate their most recent results, poster presentation time was scheduled. In addition to these formal interactions, "free time" was scheduled to allow informal discussions. Such discussions are fostering new collaborations and joint efforts in the field (program enclosed). 14. SUBJECT TERMS 20033319 16. PRICE CODE				
17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIF OF ABSTRACT	ICATION 20. LIMITATION OF ABST	TRACT



GORDON RESEARCH CONFERENCES frontiers of science

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2001 GORDON RESEARCH CONFERENCE

on Molecular Energy Transfer



FINAL PROGRESS REPORT

AFOSR F49620-00-1-0340

The Gordon Research Conference (GRC) on Molecular Energy Transfer was held at Harbortown Resort, Ventura, California, January 14-19, 2001. The conference was well attended with 89 participants (list enclosed). The attendees represented the spectrum of endeavor in this field coming from academia, industry, and government laboratories, both US and foreign scientists, senior researchers, young investigators, and students.

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I want to personally thank you for your support of this Conference. As you know, in the interest of promoting the presentation of unpublished and frontier-breaking research, Gordon Research Conferences does not permit publication of meeting proceedings. If you wish any further details, please feel free to contact me. Thank you.

Joel Bowman Conference Chair

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Distribution Unlimited

Molecular Energy Transfer

January 14-19, 2001 Harbortown Resort Ventura, CA



Contents:

- OVERVIEW, SPONSORS & SOCIAL PROGRAM
- PROGRAM
- POSTERS
- CONFERENCE HISTORY

Overview

As is customary, the meeting (which alternates every two years between Europe and the US) will cover all aspects of energy transfer, such as decomposition and reaction dynamics, intramolecular energy transfer, and energy transfer in media ranging from gas and clusters to condensed phases and interfaces. Several sessions will be devoted to new topics such as He nanodroplets, single molecule detection, etc. Oral sessions will take place in the morning and in the evening. At the beginning of each session, the session Chair will give a 20 minute perspective of the field. Each oral presentation will be 35 minutes, leaving ample time for discussion.

The conference will begin on Sunday afternoon at 4:30 PM with a reception and oral presentations at 7:30 PM. Poster sessions will take place after the evening talks on Monday - Thursday. Afternoons are free for discussions, volleyball at the beach, jogging, swimming, etc. Trips to nearby points of interest will be organized. The conference will culminate with the Thursday evening banquet, and the after dinner session in which the breadth of the field of molecular energy transfer, its modern practice and novel directions will be discussed. Departure is on Friday morning.

Application forms for the Gordon Conference must be submitted to the GRC office, P.O. Box 984, West Kingston, RI 02892-0984. Tel. 401 783-4011 (-7644 fax). Applications can also be made online by clicking the appropriate button at the bottom of this page. Early application is encouraged because the conference has usually close to the maximum allowed number of attendees. The deadline for registration at a reduced rate is 4 weeks prior to the conference. Please plan to apply by December 7, 2000. The deadline for submission of posters is December 22, 2000. We are trying to raise support for student and postdoc travel. The preliminary program is listed below. The full program with titles will be published in September.

Sponsors

- U.S. Air Force Office of Scientific Research
- U.S. Office of Naval Research
- The Gordon Research Conferences
- Gaussian, Inc.
- Spectra Physics
- Continuum Lasers

Social Program

Social Program

Tours to the Getty Museum and Whale Watching will be arranged for Tuesday afternoon. The cost will be about \$30 per trip. A sign-up sheet will be available on Sunday evening with more details.

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	Projection		
-	00 - 9:00 p.m. Registration		
6:00 p.m.	Dinner		
	Spectroscopy and Reading vin Clusters		
	Session Chair: Marsha L. Lester		
7:30 - 7:40	Conference Chairs: Opening Remarks		
7:40 - 8:00	Marsha L Lester (University of Pennsylvania) Perspective and overview		
8:00 - 8:50	Michael C. Heaven (Emory University) Non-adiabatic predissociation of Van der Waals molecules		
8:50 - 9:40	Nadine Halberstadt (Universite Paul Sabatier, Toulouse) Time-dependent study of vibrational energy relaxation in Van der Waals complexes: From the 1:1 diatomic-rare gas complex to the diatomic in a complete "solvent" shell		
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	Session Chair: Curt Wittig		
8:30	Conference Photo		
9:00 - 9:20	Curt Wittig: (University of Southern California) Perspective and overview		
9:20 - 10:10	Kaoru Yamanouchi (The University of Tokyo) Ultrafast structural deformation of small polyatomic molecules in intense laser fields		
10:10 - 10:40	Break		
10:40 - 11:30	Thomas R. Rizzo (Ecole Polytechnique Federale de Lausanne) IVR-limited unimolecular dissociation rates in state-selected HOCl and HOBr		
11:30 - 12:20	Reinhard Schinke (Max-Planck-Institüt fur Strömungsforschung) Quantum mechanical perspective of unimolecular dissociation		
12:30 - 1:30	Lunch		
2:00	Business Meeting		
Monday bine	January 15, ત્રાળો		
6:00 p.m.	Dinner		
	Photodissociation in Complexes		
	Session Chair: Jeremy M. Hutson		
7:30 - 7:50	Jeremy M. Hutson (University of Durham) Perspective and overview		
7:50 - 8:40	Robert E. Continetti (University of California at San Diego) Studies of three-body dissociation dynamics by dissociative dhotodetachment		
8:40 - 9:30	R. Benny Gerber (Hebrew University) Photochemical reactions, charge transfer and electronic energy relaxation in weakly-bound clusters		
9:30 p.m.	Poster Session I		
Trockoffy station	Danung 16: 1001 Dhogatesanegari Dynenikas		

	Session Chair: Keiji Morokuma
9:00 - 9:20	Keiji Morokuma (Emory University) Perspective and overview
9:20 - 10:10	Laurie J. Butler (The University of Chicago) Probing the dissociation dynamics of selected high-energy hydrocarbon radical isomers: Allyl, 1-propenyl and 2-propenyl
10:10 - 10:40	Break
10:40 - 11:30	Kirk A. Peterson (Washington State University) Photodissociation of halogen oxide molecules: HOCl, HOBr, and BrO
11:30 - 12:20	Jingsong Zhang (University of California, Riverside) Photodissociation dynamics of vinyl and ethyl radicals
12:30 - 1:30	Lunch
1:30 - 6:00 p.m	Optional Tours
Thesday name.	Danuery 16,2000
6:00 p.m	Dinner
	He Namodroplets
	Session Chair: Roger E. Miller
7:30 - 7:50	Roger E. Miller (University of North Carolina) Perspective and overview
7:50 - 8:40	Kenneth C. Janda (University of California, Irvine) Toward chemical reaction dynamics at 0.4 K
8:40 - 9:30	Andrej Vilesov (University of Southern California) Molecular spectroscopy in helium droplets
9:30 p.m.	Poster Session II
Wednesdbyrasi	Bimolecular Reactions
	Session Chair: Paul J. Dagdigian
9:00 - 9:20	Paul J. Dagdigian (Johns Hopkins University) Perspective and overview
9:20 - 10:10	Piergiorgio Casavecchia (Universita di Perugia) Recent progress in crossed beam studies of reaction dynamics
10:10 - 10:40	Break
10:40 - 11:30	David Manolopoulos (Oxford University) Some recent developments in chemical reaction dynamics
11:30 - 12:20	F. Javier Aoiz (Compluteuse University, Madrid) A reaction with several paths: Dynamics and stereodynamics of the O(1D)+H2 reaction
12:30 - 1:30	Lunch
Weificath), pu	n _a Anniaty 17, 2001
6:00 p.m.	Dinner
	Single=Molecule Studies of Energy-Transfer Communication Session Chair: George W. Flynn
7:30 - 7:50	George W. Flynn (Columbia University) Perspective and overview
7:50 - 8:40	Paul F. Barbara (University of Texas, Austin) Single moelcule spectroscopic studies of intramolecular energy transfer in complex systems
8:40 - 9:30	Wilson Ho (University of California, Irvine) Vibrational energy transfer in single adsorbed molecules with sub-Ångstrom resolution
	•

9:30 p.m.	Poster Session III
idiųjsiky sym _ė	damnos, 18, 2001
	Briegy Henstern-the Condensed Physe
	Session Chair: Peter J. Rossky
9:00 - 9:20	Peter J. Rossky (University of Texas, Austin) Perspective and overview
9:20 - 10:10	Gilbert M. Nathanson (University of Wisconsin, Madison) One second in the life of HCl in liquid glycerol: Solvation, dissociation, and recombination
10:10 - 10:40	Break
10:40 - 11:30	Stephen E. Bradforth (University of Southern California) The dynamics of photodetachment and photoionization in aqueous solution
11:30 - 12:20	Tim Lian (Emory University) Dynamics of molecular adsorbates on nanoparticles: vibrational relaxation, solvation and electron transfer
12:30 - 1:30	Lunch
4:00 - 6:00 p.m	Poster Session IV
Ilmusiky jum.	, Iknпину 16, 200П
6:00 p.m.	Dinner
	New Thrends in Molecular Energy Deansfer
	Session Chair: Millard H. Alexander
8:00 - 8:20	Millard H. Alexander (University of Maryland) Perspective and overview
8:20 - 9:20	Stephen R. Leone (NIST/University of Colorado) Molecular energy transfer - where are we going? From vibration-vibration to quantum information science
9:20 - 9:30	Conference Chairs: Summary Comments
Trinday ating le	mery 19, 200) t
7:30 - 8:30	Breakfast
9:00:	End of Conference; Bus Departs

Poster Sessions I and II: Displayed Monday and Tuesday

Odd numbers: Presented Monday Even numbers: Presented Tuesday

- Experimental Investigation of the Low Lying Electronic States of CH₂Cl
 <u>Aaron Potter</u>, <u>Vladimir Dribinski</u>, Andrey Demyanenko and Hanna Reisler Chemistry Department, University of Southern California
- Laser Jet Spectroscopy of Molecular Microclusters of Pyridylindoles
 Y. Nosenko and <u>A. Mordzinski</u>
 Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw
- Ab Initio Calcluations of Electronically Excited States of the CH₂Cl Radical <u>S. Levchenko</u> and A. Krylov. Chemistry Department, University of Southern California
- 4. The Infrared Spectroscopy of H-Bonded Dimers in their Ground and First Excited Singlet States Gina M. Florio, Edwin L. Sibert, III, Christopher J. Gruenloh, and Timothy S. Zwier

Purdue University, West Lafayette, IN and University of Wisconsin-Madison

- Infrared Spectroscopy of Vibrationally Excited Methanol and Some of its Isotopomers
 <u>D. Rueda</u>, O. V. Boyarkin, T. R. Rizzo
 Laboratoire de Chimie Physique Moléculaire, EPFL, Lausanne
 A. Chirokolava, D. S. Perry
 Department of Chemistry, University of Akron, Ohio
- Vibrationally Mediated Photodissociation of H₂O
 <u>Joelle Underwood</u>, Delphine Chastaing, Judson Partin, and Curt Wittig Chemistry Department, University of Southern California
- Photodissociation Dynamics of CH₂OH and its Isotopomers from the 3p_z Rydberg State <u>Feng. L</u>; Khodykin, O; Conroy D; Aristov, V; Nishimura. P; Reisler, H Chemistry Department, University of Southern California
- Mapping of the OH + CO reaction pathway throught infrared spectroscopy of the OH-CO reactant complex
 <u>Marsha Lester</u>, Bethany V. Pond, Mark D. Marshall, and David T. Anderson,
 Department of Chemistry, University of Pennsylvania
 Lawrence B. Harding and Albert F. Wagner,
 Chemistry Division, Argonne National Laboratories
- Dynamics of vibrationally mediated photodissociation of H₂O and Ar-H₂O,
 Sergey A. Nizkorodov, Michael Ziemkiewicz, Tanya L. Myers, David J. Nesbitt.
 JILA/NIST and Department of Chemistry and Biochemistry, University of Colorado,
- Emission Spectroscopy and Ab Initio Characterization of the Excited States of Allyl Iodide and Allyl Alcohol Accessed Near 200 nm <u>Brad Parsons</u> and Laurie J. Butler Department of Chemistry, The University of Chicago
- Ab initio calculation of widths of HOCl(7v_{OH}, and 8v_{OH}) resonances and comparison with experiment.
 Shengli Zou, Sergei Skokov, and Joel M. Bowman
 Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University
- 12. QUASICLASSICAL TRAJECTORY STUDY OF THE H (Cl) + HCN --> H₂ (HCl) + CN REACTION DYNAMICS AND MICROSCOPIC MECHANISM

 Diego Troya ^(a), Miguel González ^(b) *, Guosheng Wu ^(c), and George C. Schatz ^(c) *

 (a) Departamento de Química, Universidad de La Rioja,

 C/ Madre de Dios, 51. 26004 Logroño (Spain).

 (b) Departament de Química Física i Centre de Recerca en Química Teòrica,

 Universitat de Barcelona, C/ Martí i Franquès, 1. 08028 Barcelona (Spain).

 (c) Departament of Chemistry, Northwestern University, 2145 Sheridan Rd,

 Evanston IL 60208-3113 (USA).
- 13. NASCENT OH(X²Π;, v"=0-4) STATE-DISTRIBUTIONS FROM THE O(¹D)+C₂H₆, C₂H₄
 REACTIONS. A LIF AND QCT STUDY

 <u>Miguel González</u> (a) *, María P. Puyuelo (b), Jordi Hernando (a), R. Sayós (a), Pedro A. Enríquez (b), and Javier Guallar (b)

 (a) Departament de Química Física i Centre de Recerca en Química Teòrica,
 Universitat de Barcelona, C/ Martí i Franquès, 1. 08028 Barcelona (Spain)

 (b) Departamento de Química, Universidad de La Rioja,
 C/ Madre de Dios, 51. 26004 Logroño (Spain)
- Semiclassical Tunneling Splitting of the Ground State
 <u>Gennady Mil'nikov</u> and H. Nakamura
 Department of Theoretical Studies, Institute for Molecular Science, Okazaki, Japan.

- 15. The Vibrational Energy Transfer of NO(X²Π, v) to NO₂(v₃) Studied by Tme-Resolved FTIR Emission Spectroscopy Yuchuan Gong, Xiron Chen, and Brad R. Winer Department of Chemistry, University of Puerto Rico, San Juan
- 16. Unimolecular Reaction Rate Constants of NO₂ Just Above the Treshold <u>Daniil Yu Stolyarov</u> and Curt Wittig University of Southern California
- Absolute Cross Sections for Vibrational Deactivation and Electronic Quenching of the pDFB molecule
 with High Vibrational Energy
 <u>Uros S. Tasic</u> and C. Parmenter
 Department of Chemistry, Indiana University
- 18. Collisional Energy Transfer of Highly Vibrationally Excited Methyl- and Azabenzenes: Transition Probabilities and Relaxation Pathways from KCSI Experiments and Trajectory Calculations Uwe Grigoleit, Thomas Lenzer, <u>Klaus Luther</u>, Martin Muetzel, and Atsuko Takahara Institut fuer Physikalische Chemie, Universitat Goettingen, Germany
- The H + NO₂ Channels in the Photodissociation of HONO at 193.3 nm Gabriel Amaral, <u>Kesheng Xu</u> and Jingsong Zhang Department of Chemistry, University of California, Riverside
- Site-specific Photodissociation of Ethyl Iodide at 193.3 nm <u>Gabriel Amaral</u>, Kesheng Xu and Jingsong Zhang Department of Chemistry, University of California, Riverside
- Predominance of Non-Equilibrium Dynamics in the Photodissociation of Ketene in the Triplet State
 <u>A.L. Kaledin</u>, J. Seong, and K. Morokuma
 Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University
- Potential energy surfaces for the A² A state of CH-Ar <u>Galina Y. Kerenskaya</u>, Alexey L. Kaledin, and Michael C. Heaven Department of Chemistry, Emory University, Atlanta
- Kinetic spectroscopy of NCl
 A. V.Komissarov, M. C. Heaven
 Department of Chemistry, Emory University, Atlanta
- Dynamics of Rovibrational Transfer in Li₂-Ne Collisions
 Kristin M. Burgess, Amy M. Schneider, Troy N. Stephens, Alena Widman, and <u>Brian Stewart</u> Chemistry Department, Wesleyan University
- 25. The photodissociation of CH₃SCH₃ and CD₃SCD₃ in the first absorption band studied by velocity map imaging and REMPI F. J. Aoiz, ¹ L. Banares, ¹ B. Martinez-Haya, ² P. Quintana, ¹ and E. Verdasco ¹ 1. Departamento de Quimica Fisica, Facultad de Quimica and CAI de Espectroscopia. Universidad Comlutense. 28040 Madrid, Spain 2. Departamento de Ciencias Ambientales, Facultad de Ciencias Experimentales, Universidad Pablo de Olavide, Ctra. de Utrera, km, 1, 1013 Sevilla, Spain
- Combining hexapoles with stimulated emission pumping.
 Daniel Matsiev, and <u>Alec M. Wodtke</u>
 UC Santa Barbara, Department of Chemistry & Biochemistry, Santa Barbara, CA
- Spectra of water dimer and trimer from ab initio potentials
 <u>Krzysztof Szalewicz</u>
 Department of Physics and Astronomy, University of Delaware

- Electronic Spectroscopy and State-Resolved Photodissociation of Jet-Cooled Vinyl Radical <u>M.B. Pushkarsky</u>, A. Mann and C. B. Moore Laser Spectroscopy Facility, Dpartment of Chemistry, The Ohio State University
- 29. Jeremy Hutson
- 30. John Mccaffrey

Poster Sessions III and IV: Displayed Wednesday and Thursday

Odd numbers: Presented Wednesday Even numbers: Presented Thursday

- Low-temperature kinetics of reactions of C₂H and OH radicals with selected hydrocarbons
 <u>A. B. Vakhtin</u>, S. Lee, D. E. Heard(*), I. W. M. Smith(*), and S. R. Leone
 <u>JILA</u>, NIST and University of Colorado, Department of Chemistry and Biochemistry
 (*) JILA Visiting Fellow
- Photodissociation of ICN in Cyclohexane: A Study of Solvent Effects on Reaction Dynamics
 <u>Amy C. Germaine</u>, Victor A. Lenchenkov, Victor H. Vilchiz, Jeremiah A. Kloepfer, and Stephen E.
 Bradforth
 Chemistry Department, University of Southern California
- Rotationally Inelastic Collisions of Highly Rotationally Excited Free Radicals: CH(A²Δ) and CN(A²Π)
 B.Nizamov and P.J. Dagdigian.
 Chemistry Department, The Johns Hopkins University
- Femtosecond Dynamics of ICl (CO₂)_n Clusters
 <u>Django Andrews</u> and Carl Lineberger
 JILA, University of Colorado, Boulder, Colorado
- Dynamics of Harpooning in Li..FCH₃ van der Waals complex
 A.J. Hudson, F.Y. Naumkin, H.B. Oh, <u>S.R. Raspopov</u> and J.C. Polanyi Department of Chemistry, University of Toronto
- 6. Inter- and intramolecular energy transfer of diphenylpolyenes in solution explored by fs-fluorescence up-conversion.
 C. Grimm, J. Schroeder, <u>T. Steinel</u> and J. Troe IPC, University of Goettingen
- Theoretical studies of the product translational energy distributions in the F + HD --> HF + D reaction <u>Yi-Ren Tzeng</u> and Millard H. Alexander Department of Chemistry and Biochemistry and Chemical Physics Program, University of Maryland
- Vibrational Self-consistent Field Approach to Anharmonic Spectroscopy of Molecules in Solids: Application to I₂ in Argon Matrix
 Zsolt Bihary, Benny Gerber, and Ara Apkarian
 University of California, Irvine, USA and Hebrew University, Israel
- Comparison of the Reactivity of the Symmetric and Antisymmetric Stretch of CH₄ on the Reaction of Cl
 (²P_{3/2}) + CH₄
 Sangwoon Yoon, Sarah Henton, Aleks Zivkovic, and F. Fleming Crim
 Department of Chemistry, University of Wisconsin-Madison
- Full-dimensional IVR calculations on medium-sized organic molecules and their comparison to experiment: Pyrrole and Triazine.
 Ryan Pearman and Martin Gruebele Department of Chemistry, University of Illinois

- The effect of Ar atoms on the dynamics of the O(³P) + HCl reaction <u>Lichang Wang</u>, and Anne B. McCoy Department of Chemistry, The Ohio State University
- Time-resolved studies of energy transfer from a vibrationally excited I₂- chromophore into surrounding Ar or CO₂ clusters
 Roland Wester, Alison V. Davis, Arthur E. Bragg, Daniel M. Neumark

Roland Wester, Alison V. Davis, Arthur E. Bragg, Daniel M. Neumard Department of Chemistry, University of California, Berkeley

13. Reduced dimensionality quantum calculations of the Cl + CH₄ reaction and a prediction on the effect of bend excitation on the HCl rotational distribution. Sergei Skokov and <u>Joel M. Bowman</u> Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University,

14. THEORETICAL STUDY OF THE N(⁴S) + O₂(X³Σ_g⁻) --> NO(X²Π) + O(³P) REACTION. FROM THE ELECTRONIC STRUCTURE TO THE RATE CONSTANT. Carolina Oliva, Miguel González, and R. Sayós Departament de Química Física i Centre de Recerca en Química Teòrica C/ Martí i Franqués 1, Barcelona (Spain)

15. Ab initio ³A" ground potential energy surface for the O(³P) + N₂O reaction and kinetics study Rosendo Valero, R. Sayós, and Miguel González Departament de Química Física i Centre de Recerca en Química Teòrica, Universitat de Barcelona. C/ Martí i Franquès, 1. 08028 Barcelona, Spain.

16. Ab initio and VTST kinetics study of the N(¹D)+O₂(X³Σ_g) reaction including excited PES Irene Miquel, R. Sayós *, and Miguel González * Departament de Química Física i Centre de Recerca en Química Teòrica, Universitat de Barcelona. C/ Martí i Franquès, 1. 08028 Barcelona, Spain.

Vibrational spectroscopy and intermolecular vibrational energy transfer for glycine molecule and its complex with water.
 Galina M. Chaban, R. Benny Gerber
 NASA Ames Research Center, Moffett Field, CA, and Hebrew University, Israel

Relaxation Processes in Multimolecular Systems
 <u>Eduard Zenkevich</u>
 Laboratory of Molecular Photonics, Institute of Molecular and Atomic Physics, Minsk, Belarus

NO(v)-O vibrational energy transfer and its photochemical role in the thermosphere
 <u>Eunsook S. Hwang</u>¹ and James Dodd²
 (1)Stewart Radiance Laboratory, Bedford, MA, and (2) Air Force Research Lab, Hanscom AFB

Recent Studies of OH(v) Dynamics
 <u>James A. Dodd¹</u> and Eunsook S. Wang²
 (1) Air Force Research Laboratory, Hanscom AFB, MA; and Stewart Radiance Laboratory, Bedford, MA

 Quantum Dynamical Studies of Atom-Diatom Insertion Reactions <u>Jean-Michel Launay</u> and Pascal Honvault Université de Rennes, UMR 6627 du CNRS, Rennes, France

Li + HF: A Case Study to Develop Novel Computational Technologies for Reactive Scattering
 Antonio Lagana
 Universita di Perugia, Dipartimento di Chimica, Italy

23. Theoretical Study of Scanning tunneling Miscroscope Induced Desorption of Benzene from Si(100)

Surface
Saman Alavi, Roger Rousseau and Tamar Seideman
National Research Council of Canada, Steacie Institute for Molecular Sciences, Ottawa, Canada

- Isotopically Selective Collisonal Vibrational Energy Transfer Oleg Boiarkine and T.R. Rizzo EPFL, LCPM, DC. EPFL, Lausanne, Switzerland
- 25. The Relavative Distributions of State-to-State Inelastic Scattering Cross Sections of S₁ trans-Glyoxal Demonstrate a Center-of-Mass Momentum Correlation Samuel M. Clegg, Mariana Duca and Charles S. Parmenter Sandia National Laboratories, Livermore, CA
- 26. The Dynamics and Stereodynamics of Four-Body Chjemical Reactions by Quasiclassical Trajectory Methods on Ab Initio Potential Energy Surfaces <u>Jesus Santamaria</u> Universidad Complutense de Madrid, Departamento de Quimica Fisica, Facultad de Quimica, Madrid, Spain
- 27. Energy transfer from excited NH₂ in the presence of NO, studied by time-resolved FTIR emission spectroscopy Timothy P. Marcy, Dwayne E. Heard and Stephen R. Leone JILA/NIST and Department of Chemistry and Biochemistry, University of Colorado
- 28. Trajectory Surface-Hopping Study of the $I(^2P_{3/2}) + O_2(a^1\Delta_g) --> I(^2P_{1/2}) + O_2(X^3\Sigma_g)$ Energy Transfer Process A.L. Kaledin, M.C. Heaven, and K. Morokuma Cherry L. Emerson Center for Scientific Computation and Dept. of Chemistry, Emory University
- A quasi-classical trajectory study of the H+N₂O reaction
 J. F. Castillo, F. J. Aoiz, <u>L. Banares</u>, and J. Santamaria
 Departamento de Quimica Fisica, Facultad de Quimica and CAI de Espectroscopia. Universidad Comlutense. 28040 Madrid, Spain
- 30. New 3-D potential energy surface for the He-CO system George C. McBane and Kirk Peterson Department of Chemistry, The Ohio State University and Washington State University
- 31. Vibrational effects in collision-induced dissociation dynamics of the Ar₂+ + Ar/Ne systems
 J. Scott Miller, ¹ Rainer Dressler, ¹ Yu-hui Chiu, ² and Dale J. Levandier²
 (1) Air Force Research Lab, Hanscom AFB, and (2) Boston College, Institute of Scienctific REsearch, Newton.

Conference History

Continuing progress in our understanding of molecular energy transfer, and the importance of this process, have provided the impetus for a series of conferences on this topic, dating back to 1969. The conferences have taken place biennially, in alternation between a Gordon Research Conference (GRC) on Molecular Energy Transfer and a European Conference on Molecular Energy Transfer (COMET). This alternation underlines the international aspect of the field and provides a regular channel for exchange between scientists in North America and Europe. The previous GRC/COMET conferences in this series, sites, and organizers are listed below.

Date	Conference	Site	Conference Chair(s)
1969	rore T	Medy Hampshite	Definer Steinfeldland Charles Pannenter
1971	COMET =	Cambridge (UK)	Amiliony Galleric Control of the Con
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1980	HGRC : - :	New isomposities	Emie Wenz and George Scharz
1001	COMM	Niffmegen (Meinerander)	ling Reps
19932		+ New Bampsinie	David King and John Stephenson,
1995	COMED	Z Kuosia ikaw (Germay).	Hens Joachin Wemer and Reter Andreson
1997	GRC -	Venting, CA	Marsha Leafer and Millard Alexander, 2001
1000	The state of the s	A graty = 2	Antono Lagana and P. Casavecchia
2001	GRC +	Wonning CARL H. T.	i Banna Reisler and Joel Bownian
2003	COME	Spain	Filavier Adizard Miguel Convalez



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MOLECULAR ENERGY TRANSFER

FOUR POINTS SHERATON: HARBORTOWN (14-Jan-01) - (19-Jan-01)

NOTE: Receipt of Application does not guarantee acceptance to a Conference. Applications are reviewed by the Conference Chair. If the Chair approves your application, you become Accepted, and a registration packet will be mailed immediately. Please allow 3-5 days for your registration to reach you by mail once your name appears. When your registration packet has been received back in our office, you become Registered.

Only those who have been Accepted or Registered will have their names listed below. Names of people who have only applied and have yet to be accepted will NOT appear.

Nomo	Organization	Participation	Status
Name SAMAN ALAVI	NATIONAL RESEARCH COUNCIL OF CANADA	Poster Presenter	Registered
MILLARD H ALEXANDER	UNIVERSITY OF MARYLAND	Speaker	Registered
DJANGO H ANDREWS	UNIVERSITY OF COLORADO	Poster Presenter	Registered
	UNIVERSIDAD COMPLUTENSE	Speaker	Registered
FRANCISCO J AOIZ LUIS BANARES	UNIVERSIDAD COMPLUTENSE	Poster Presenter	Registered
PAUL F BARBARA	UNIVERSITY OF TEXAS AT AUSTIN	Speaker	Registered
ZSOLT BIHARY	UNIVERSITY OF CALIFORNIA	Poster Presenter	Registered
OLEG V BOLARKINE	SWISS FED. INSTIT. OF TECH.	Poster Presenter	Registered
JOEL BOWMAN	EMORY UNIVERSITY	Chair	Registered
STEPHEN E BRADFORTH	UNIVERSITY OF SOUTHERN CALIFORNIA	Speaker	Registered
LAURIE J BUTLER	THE UNIVERSITY OF CHICAGO	Speaker	Registered
PIERGIORGIO CASAVECCHIA	UNIVERSITA DI PERUGIA	Speaker	Registered
GALINA M CHABAN	NASA	Poster Presenter	Registered
STEVE CHAMBREAU	UNIVERSITY OF CALIFORNIA, RIVERSIDE	Poster Presenter	Registered
DELPHINE CHASTAING	UNIVERSITY OF SOUTHERN CALIFORNIA	Attendee	Registered
	SANDIA NATIONAL LABORATORIES	Poster Presenter	Registered
SAMUEL M CLEGG	UNIV. OF CALIFORNIA, SAN DIEGO	Speaker	Registered
ROBERT E CONTINETTI	JOHNS HOPKINS UNIVERSITY	Speaker	Registered
PAUL J DAGDIGIAN	AIR FORCE RESEARCH LABORATORY	Poster Presenter	Registered
JAMES A DODD	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
VLADIMIR L DRIBINSKI	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
LIN FENG	PURDUE UNIVERSITY	Poster Presenter	Registered
GINA M FLORIO	COLUMBIA UNIVERSITY	Speaker	Registered
GEORGE W FLYNN	HEBREW UNIVERSITY	Speaker	Registered
BENNY GERBER	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
AMY C GERMAINE	UNIVERSITY OF PUERTO RICO	Poster Presenter	Registered
YUCHUAN GONG	UNIVERSITY OF BARCELONA	Poster Presenter	Registered
MIGUEL GONZALEZ	CNRS-UNIVERSITE PAUL SABATIER	Speaker	Registered
NADINE HALBERSTADT	UNIVERSITY OF CALIFORNIA, SANTA BARBARA	Attendee	Registered
NILS HANSEN	EMORY UNIVERSITY	Speaker	Registered
MICHAEL C HEAVEN	UNIVERSITY OF CALIFORNIA	Speaker	Registered
WILSON HO	UNIVERSITY OF DURHAM	Speaker	Registered
JEREMY M HUTSON	UTAH STATE UNIVERSITY	Poster Presenter	Registered
EUNSOOK S HWANG	UNIVERSITY OF CALIFORNIA, IRVINE	Speaker	Registered
KENNETH C JANDA	EMORY UNIVERSITY	Poster Presenter	Registered
ALEXEY L KALEDIN	EMORY UNIVERSITY	Poster Presenter	Registered
GALINA KERENSKYA	EMORY UNIVERSITY	Poster Presenter	Registered
ANATOLY V KOMISSAROV	UNIVERSITE DE RENNES	Poster Presenter	Registered
JEAN-MICHEL LAUNAY	NIST/ UNIVERSITY OF COLORADO	Speaker	Registered
STEPHEN LEONE	UNIVERSITY OF PENNSYLVANIA	Speaker	Registered
MARSHA I LESTER	BOSTON COLLEGE INSTITUTE FOR SCIENTIFIC RESEARCH	Poster Presenter	Registered
DALE J LEVANDIER	UNIVERSITY OF SOUTHERN CALIFORNIA	Poster Presenter	Registered
SERGEY V LEVCHENKO	EMORY UNIVERSITY	Speaker	Registered
TIANQUAN LIAN	UNIVERSTIY OF COLORADO, BOULDER	Attendee	Registered
CARL LINEBERGER	UNIVERSITI OF COLURADO, BOOLDER		J

KLAUS H LUTHER DAVID MANOLOPOULOS TIMOTHY P MARCY DANIEL V MATSIEV GEORGE C MCBANE JOHN MCCAFFREY ANNE B MCCOY ROGER E MILLER ANDRZEJ MORDZINSKI KEIJI MOROKUMA **GILBERT M NATHANSON BORIS R NIZAMOV** SERGUEI A NIZKORODOV **CHARLES PARMENTER** BRADLEY F PARSONS RYAN PEARMAN KIRK A PETERSON ELENA YU POLYAKOVA AARON B POTTER MICHAEL B PUSHKARSKY SERGUEI A RASPOPOV HANNA REISLER THOMAS R-RIZZO PETER J ROSSKY DAVID RUEDA REINHARD SCHINKE TOBIAS STEINEL **BRIAN A STEWART** DANIIL YU STOLYAROV KRZYSZTOF SZALEWICZ UROS S TASIC YI-REN TZENG JOELLE S UNDERWOOD ANDREI VAKHTIN MARC C VAN HEMERT ANDREJ VILESOV LICHANG WANG ROLAND WESTER **CURT WITTIG** ALEC WODTKE KESHENG XU KAORU YAMANOUCHI SANGWOON YOON JINGSONG ZHANG

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